

Nuclides 2000 – Die Nuklidkarte auf CD-ROM

Mit dem Softwarepaket „Nuclides 2000“ steht eine elektronische Nuklidkarte auf CD-ROM für Microsoft Windows Betriebssysteme zur Verfügung, die umfangreiche physikalische und radiologisch relevante Basisinformationen und -daten zu den bekannten Nukliden bereit stellt. Zudem bietet Nuclides 2000 für eine Reihe von Anwendungen Programme an, die mittels interaktiver Benutzerführung eine schnelle und gesicherte Berechnung der gesuchten Daten ermöglichen.

Das Daten- und Programmangebot wird durch Informationen in Form von Beiträgen zur Geschichte der Radioaktivität und Radiochemie sowie physikalisch interessanten Themen – wie C14-Datierung und Bildung von ^{44}Ti in einer Supernova – sowie durch eine Link-Sammlung von Internet-Adressen ergänzt.

Als detaillierte Datenbank kann Nuclides 2000 in Lehre, Forschung und Anwendung Einsatz finden.

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Nuclides 2000: An Electronic Chart of the Nuclides on CD-ROM

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Introduction

Do you have a nuclide chart hanging in your office or nearby? If so, you will know the usefulness of these ‘collectors items’ in which radionuclides are displayed according to the number of protons Z and neutrons N in their nucleus. In addition to giving the most important basic nuclear data, this arrangement, originally proposed by Segrè, allows one to trace out decay and reaction paths qualitatively.

You will also be very aware that these charts are of limited use with regard to the amount of data that can be shown. More over, one invariably has to go a step further and make calculations with this data. Until now, the solution was to resort to large computer codes or if this takes too long, to write a computer program to solve the decay equations. Another possibility would be to have the calculations done by an expert.

These problems have now been overcome with the development of Nuclides 2000 [1]. With this new “Electronic” Chart, there is basically no limitation on the amount of data that can be stored and shown for any particular nuclide. More importantly, one can now do calculations quickly, reliably, using qualified data in a user-friendly environment. Tedious calculations are now redundant with this package. Through the **Nuclide Explorer**, the backbone of the Nuclides 2000 software, the user has access to powerful navigational, informational, and calculational interfaces. These allow fast identification of the particular nuclide(s) of interest, a summary of the basic nuclear and radiological data, and calculations using this data.

Other features of Nuclides 2000 include articles and weblinks. In the **Articles**, various aspects of radioactivity and radiation ranging from radiocarbon dating to the formation of ^{44}Ti in supernova. There are arti-

cles covering the history of radioactivity and radiochemistry and descriptions of all the chemical elements. The articles database is fully indexed and can be searched for keywords. Use of wildcards and jokers is allowed in the keyword selection. The displayed topic contains the keyword highlighted wherever it appears in the text. The **Online Features** allow the user to access websites of related interest. A browser window opens with the Nuclides 2000 homepage. Sites are classified under the general headings: Glossary of Nuclear Science, Classical Scientific Papers, Historical, People, New Elements, Origin of Nuclides, Introduction to Radiation and Radioactivity, Applications of Radionuclides, Archaeology, Radon, Nuclear Data, Organizations etc.

Nuclides 2000 is aimed at specialists who require detailed technical information such as activities, gamma emission rates, gamma dose rates, radiotoxicities, ALIs, etc. On the market for a few months, Nuclides 2000 is already being used on a daily basis by scientists in the mainstream nuclear industry, regulatory authorities, nuclear medicine, radiology, and in hospitals. As an educational tool, the program is of interest for educators and students.

Nuclides 2000 has been developed within the Institute for Transuranium Elements’ activities in establishing an actinide research reference centre. Other activities within this “Actinide Information Centre” include the development of a nuclear materials database to establish the origin of nuclear materials and a materials database for Accelerator Driven Systems (ADS). Further information can be found on the Institute website at <http://itu.jrc.cec.eu.int/> and on the Nuclides 2000 website at <http://www.nuclides.net/>.

Navigational, informational, and calculational aspects of the program are now described in more detail.

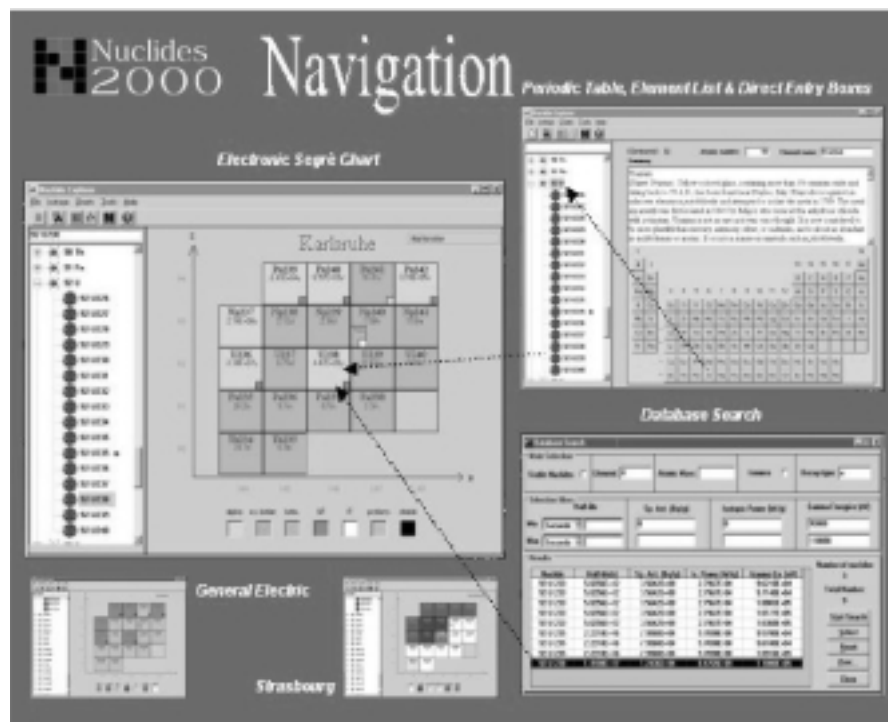


Fig.1: Selection of a chemical element from the periodic table leads to a display of isotopes in the element list box. On selection of a particular isotope, the location of the isotope in the Segrè (nuclide) chart is shown. Nuclides can also be found from the direct entry box or from the database search engine (see figure). Colours indicate the mode of decay, as in the Karlsruhe (main window) and Strasbourg (inset) charts, or half-lives as in the General Electric (inset) and JAERI charts. There is also a option to "Build-your-own" chart.

Nuclide Explorer

Navigation

Following the recent discovery of elements 114, 116, 118, there are now 115 known chemical elements (elements 113, 115, 117 are not yet known). Elements can have many isotopes, most of which are unstable. In general these isotopes are known as nuclides. The heart of the Nuclides 2000 program is the Nuclide Explorer which provides fast access to the nuclear and radiological data on more than 2600 nuclides. It also allows the user to do calculations with this data. Because of the large number of nuclides, navigation through a chart of the nuclides is more complicated than navigation through the periodic table of the elements. For this reason, the starting window shown in the Nuclide Explorer contains a periodic table as shown in fig.1. Once the element has been selected, a list of all isotopes is given in the element list box. On selection of a particular isotope, the main frame shows the location of this isotope in the Segrè or nuclide chart. Alternatively, the database can be searched to find nuclides with particular characteristics. Comprehensive Boolean search tasks can be performed. Searches can also be made on the decay type such as α ; β^- ; β^+ ; n (beta delayed neutron emission); etc.

The use of colours in these charts is to denote the fact that the nuclide is unstable (radioactive) and decays by a particular process. This is the case in the Karlsruhe [2] and Strasbourg Charts [3]. In the case of the General Electric [4] and JAERI [5] charts, the colours are used to indicate the half-lives of the nuclides. The colour scheme can be chosen directly from the taskbar. In addition, a "personal" colour scheme can be created and used.

Data Sheets

The radioactive decay data used in NUCLIDES 2000 is based on the Joint Evaluated File (JEF) version 2.2. Radiological data such as the effective dose coefficient is from the ICRP 68. The present version of the program contains decay data on more than 2600 radionuclides with more than 70000 corresponding gamma energies and emission probabilities.

In the *Data Sheets* (see fig.2), the information given consists of half-life, atomic weight, number of decay modes, branching ratios, decay energies, daughter products, mean decay energies per decay, discrete energies and emission probabilities for gammas, alphas etc., and radiotoxicity data. The source of this data is also given. From this basic data, various derived quantities

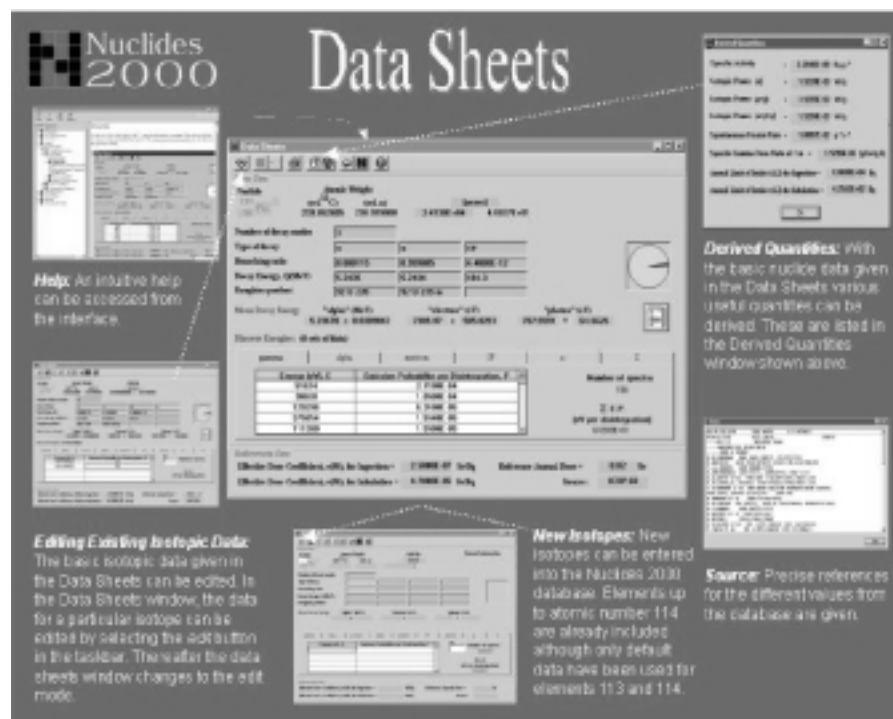


Fig.2: The Data Sheets window provides comprehensive decay and radiological data such as half-life, modes of decay, branching ratios, mean decay energies, discrete energies and emission probabilities for gammas, alphas etc., and radiotoxicity data. In the data Source, precise references are given. In the Derived Quantities, secondary quantities such as specific activity, isotopic powers, specific gamma dose rate constant, and ALI values are given. Isotope data can be Edited and New Isotopes inserted in a personal database.

can be obtained such as specific activity, isotopic powers, spontaneous fission rate, specific gamma dose rate constant at 1m, annual limits of intake (see *Derived Quantities* window). Data on elements up to atomic number 114 are included although only default data have been used for elements 113 and 114. For any element in the database, isotopes can be added and their data edited.

Decay Calculations

Through the decay calculations (see fig. 3), one can investigate the *Full Decay Scheme* of any radionuclide to obtain the numbers of atoms, masses, activities etc. accounting for all the daughters, starting from an initial mass or activity of the parent nuclide. Within the program, the Bateman equations are solved exactly accounting for multiple "chains" due to branching. The results of a decay calculation are summarised in the main window shown in fig.3. The user can investigate multiple chains due to branching by looking into the *Details*. To limit the number of chains taken into account, the variable Min.Prod can be set. This variable is the product of the branching ratios of a linear chain. The smaller this value is – the less important is the chain. If Min.Prod is set to zero, all chains will be evaluated. The default value is set to 1E-4 and is for most purposes sufficient. The variable No.Chains gives information on the number of linear

chains with the product of their branching ratios greater than Min.Prod.

In the *Options*, the user can specify which properties are to be shown in the main window results. Default values are numbers of atoms, masses, activities, gamma emission rate, gamma dose rate. Other possibilities include half-life, branching ratios, decay modes, spontaneous fission rate, isotopic powers, inhalation and ingestion radiotoxicities etc.

By specifying the distance, the specific gamma dose rate of the parent and daughters is calculated assuming a point source. By increasing the number of timesteps, calculations are performed at discrete times. From this, a *Plot* of the numbers, masses, activities etc can be made. Finally a *Segrè plot* of the decay chain is shown. Results can be cut & pasted into other applications.

Fields of application of Nuclides 2000 range from health physics, nuclear medicine, nuclear safeguards, to radionuclide dating, spent fuel characterisation, and astrophysics. We describe briefly two such applications.

Applications of Nuclides 2000

"Age" Determination of Plutonium Particles

At the Institute for Transuranium Elements, a range of analytical techniques is

being developed for verification and detection purposes to check nation state compliance with their non-proliferation commitments [6]. As part of these activities, a technique is being developed to determine the "age" of plutonium particles [7]. The "age" of a particle is defined as the time elapsed since the last chemical separation of daughter nuclides from the parent. The particles to be analysed can be obtained from the environment or from "swipes" taken at nuclear installations where clandestine activities are suspected. In view of the pending international agreement to stop the production of weapon materials, the age of such "suspected" particles is of course of great interest for verification purposes. For bulk samples, gamma spectroscopy can be used. However, for very small particles, because of the low activity, this technique is impossible.

Fresh plutonium particles will in general contain the isotopes ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu in different amounts, depending on the production route. With time, these nuclides decay to ^{234}U , ^{235}U , ^{236}U , ^{241}Am , ^{238}U respectively. By determining the ratios of the parent to daughter ($^{238}\text{Pu}/^{234}\text{U}$, $^{239}\text{Pu}/^{235}\text{U}$, $^{240}\text{Pu}/^{236}\text{U}$, $^{241}\text{Pu}/^{241}\text{Am}$, $^{242}\text{Pu}/^{238}\text{U}$) one can deduce the elapsed time and therefore the age of the particle. Because these ratios are measured by secondary ion mass spectrometry (SIMS), one cannot obtain the ratio $^{241}\text{Pu}/^{241}\text{Am}$. In addition, if the particle has some uranium contamination, one cannot use the ratio $^{242}\text{Pu}/^{238}\text{U}$. This leaves the three ratios $^{238}\text{Pu}/^{234}\text{U}$, $^{239}\text{Pu}/^{235}\text{U}$, $^{240}\text{Pu}/^{236}\text{U}$ which are suitable for age determination. The correlation between the atom ratios and the age as calculated using Nuclides 2000 is shown in fig. 4. The time scale of interest is in the range 1-50 years.

In 1994, officials at Munich Airport, seized a suspect case of luggage. The case was delivered to the ITU and was found to contain a sealed package in which several hundred grams of a radioactive powder had been concealed. The initial chemical analysis showed the powder to consist of a mixture of the oxides of plutonium and uranium. SEM examination showed that this was not a homogeneous powder sample, but was a mixture of three distinct components characterised by their morphology and chemical composition. In this micrograph (Sample F19A, fig. 4a) the different components can be identified as (1) plutonium oxide (PuO_2) in the form of small flat platelets forming the largest fraction of the mixture analysed, (2) plutonium oxide (PuO_2) particles with a rod-shaped form, (3) and Uranium oxide (U_3O_8) particles.

The correlation between the age of a particle and the Pu/U atom ratio was obtained with Nuclides 2000. The results are

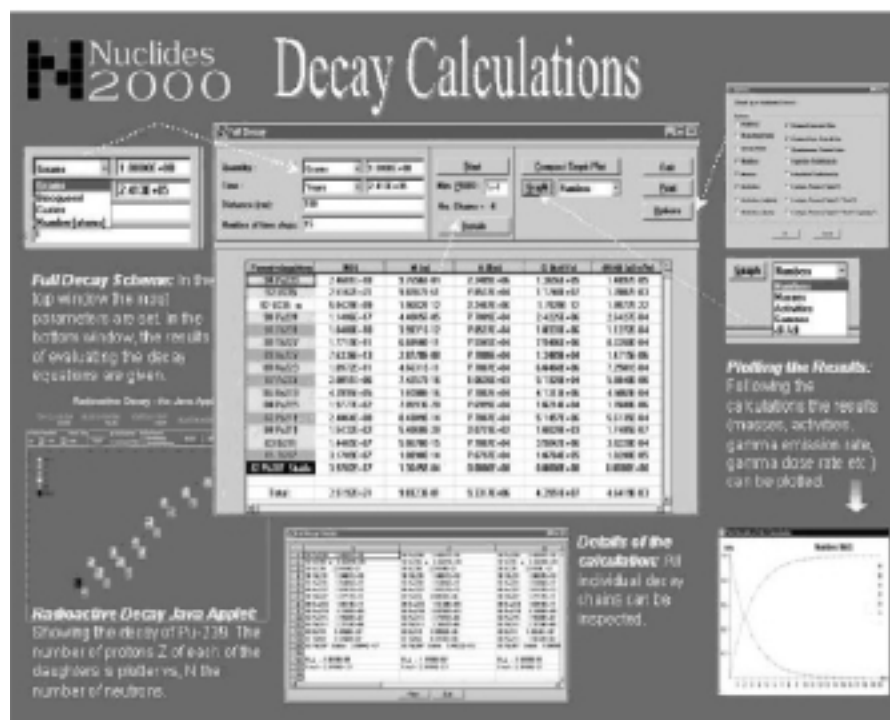


Fig.3: From the exact solution of the Bateman equations, the Decay Calculations window lists the numbers, masses, activities, gamma emission rates, gamma dose rates, etc. The actual quantities to be listed can be selected from the Options. Decay chains resulting from branching are given in the Details. The results can be Plotted directly, or cut & pasted into other applications. The nuclide decay can also be viewed in the Segrè plot.

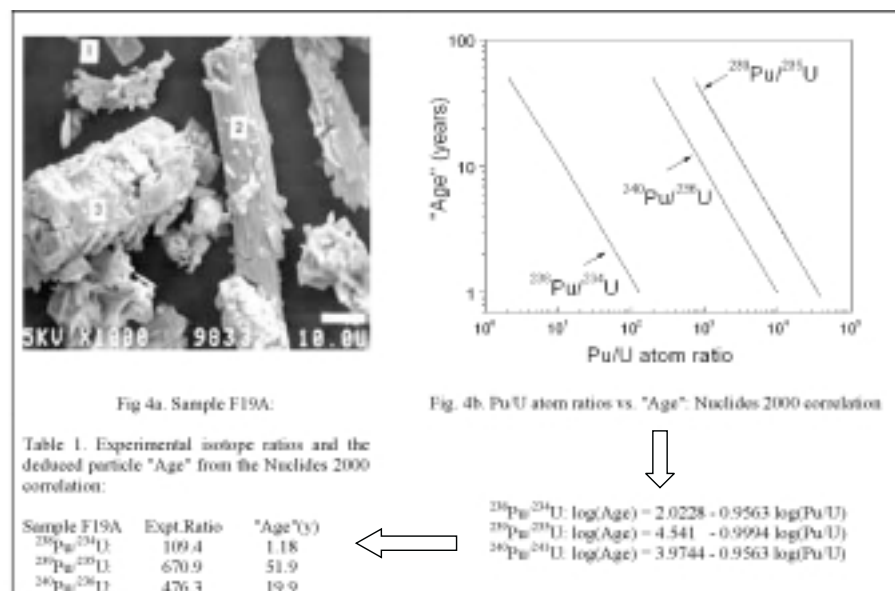


Fig. 4a/b Application of Nuclides 2000 to "Age" determination of plutonium particles. Since the uranium contamination is significant in sample F19A, the ages determined from the ratios disagree largely. The most accurate value of 19.9 y is expected from the $^{240}\text{Pu}/^{236}\text{U}$ ratio since there is no ^{236}U present in natural uranium.

shown in fig. 4b. Since the uranium contamination is significant, the ages determined from the ratios disagree largely. The most accurate is expected from the $^{240}\text{Pu}/^{236}\text{U}$ ratio, i.e. 19.9 y, since there is no ^{236}U present in natural uranium.

^{213}Bi "milking" from ^{225}Ac for cancer treatment

In alpha-immunotherapy [8], antibodies are labelled with relatively short-lived alpha emitters. Specifically targeted cancer cells are then destroyed by local deposition of energy. Of particular interest is the nuclide ^{213}Bi for this purpose. Actually ^{213}Bi is mainly a beta emitter with half-life of 46 m. This nuclide decays however to ^{213}Po , a very lived (half-life 4.2 μs) nuclide, which itself decays by alpha emission. So effectively ^{213}Bi is an alpha emitter with a half-life of 46m.

^{213}Bi is produced by the decay of the more readily available ^{225}Ac . However, before the Bi isotope can be used, it has to be eluted ("milked") from the ^{225}Ac "cow".

Once the ^{213}Bi has been separated, it starts to grow in again due to the decay of the ^{225}Ac .

The activity of the ^{225}Ac cow is typically 1GBq (27 mCi) when delivered to the Institute. By the time they arrive, the equilibrium composition of ^{213}Bi has been reached and the samples can be milked. Thereafter the Bi starts to grow in again. How often can the Ac sample be milked to obtain the maximum amount of ^{213}Bi ?

The growth of ^{213}Bi in Ac can be seen in fig. 5. It can be seen that after approximately 3h, more than 90% of the maximum value has been reached. After this time, the ^{225}Ac cow can again be milked.

References

[1] J. Magill, Nuclides 2000: An Electronic Chart of the Nuclides on CD-ROM, European Commission 1999, Institute for Transuranium Elements, Karlsruhe, Germany, ISBN 92-828-6512-6, EUR 18737 EN.

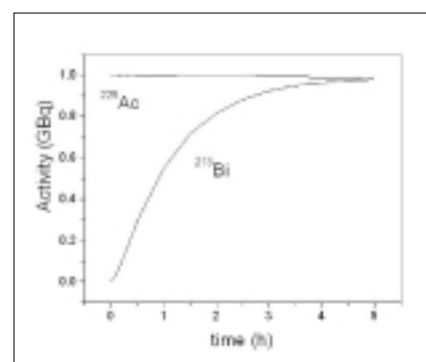


Fig. 5. In-growth of ^{213}Bi from the ^{225}Ac "cow" using Nuclides

The package with single user licence costs EUR 260. For further information, see the Nuclides 2000 website at <http://www.nuclides.net>.

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[3] Chart of the Nuclides – Strasbourg 1992, M.S. Antony, Centre de Recherches Nucléaires et Université Louis Pasteur, Strasbourg, France.

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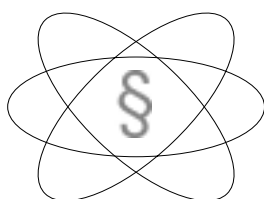
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[8] Institute for Transuranium Elements Annual Report EUR 19054 EN, 1999, p.63, for a summary of activities. See also the Institute website at <http://itu.jrc.cec.eu.int/> under Publications, Annual Report 1999, Alpha-Immunotherapy. □

Anzeige



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